

Triazole-Diindolylmethane Conjugates as New Antitubercular Agents: Synthesis, Bioevaluation and Molecular Docking

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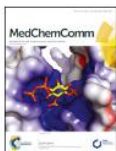
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Abstract

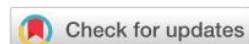
We have described the synthesis of novel triazole incorporated diindolylmethanes (DIMs) using molecular hybridization approach and their *in vitro* antitubercular activity against *Mycobacterium tuberculosis* H37Ra (ATCC 25177) both in active and dormant state. Among all the synthesized conjugates, the compounds **6b**, **6f**, **6l**, **6n**, **6q**, **6r** and **6s** displayed good antitubercular activity against both active and dormant *Mtb* H37Ra strain. The compound **6l** exhibited good antitubercular activity against *Mtb* H37Ra dormant with IC₅₀ value 1 µg/mL and IC₉₀ (MIC) value 3 µg/mL. The compounds **6b**, **6l** and **6r** displayed good antitubercular activity against *Mtb* H37Ra active with IC₅₀ values 2.19, 1.52 and 0.22 µg/mL respectively. The compounds **6b**, **6h**, **6l** and **6s** displayed more than 70% inhibition towards *B. subtilis* strain against Gram-positive bacteria at 3µg/mL. The molecular docking study shows the binding modes of the titled compounds in active site of DprE1 enzyme and was helped to launch a structural basis for the inhibition of *Mycobacteria*.

Keywords: Antitubercular activity; Diindolylmethanes; 1,2,3-Triazoles; Molecular docking; Molecular hybridization



From the journal:
MedChemComm

Triazole–diindolymethane conjugates as new antitubercular agents: synthesis, bioevaluation, and molecular docking†



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Abstract

We describe the synthesis of novel triazole-incorporated diindolymethanes (DIMs) using a molecular hybridization approach. The *in vitro* antitubercular activity of the DIMs against *Mycobacterium tuberculosis* H37Ra (ATCC 25177) was tested in the active and dormant state. Among all the synthesized conjugates, the compounds **5h**, **6f**, **6l**, **6n**, **6o**, **6r**, and **6s** displayed



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MedChemComm

Continued as: RSC Medicinal Chemistry

Scopus coverage years: from 2010 to 2019

(coverage discontinued in Scopus)

Publisher: Royal Society of Chemistry

ISSN: 2040-2503 E-ISSN: 2040-2511

Subject area: Pharmacology, Toxicology and Pharmaceutics: Pharmaceutical Science Chemistry: Organic Chemistry

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